

A Proposed Route to Thin Film Crystal Si Using Biaxially Textured Foreign Template Layers

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ABSTRACT

We have developed a new approach to growing photovoltaic-quality crystal silicon (c-Si) films on glass. Other approaches to film c-Si focus on increasing grain size in order to reduce the deleterious effects of grain boundaries. Instead, we have developed an approach to align the silicon grains biaxially (both in and out of plane) so that 1) grain boundaries are "low-angle" and have less effect on the electronic properties of the material and 2) subsequent epitaxial thickening is simplified. The key to our approach is the use of a foreign template layer that can be grown with biaxial texture directly on glass.

1. Objectives

A critical goal of the Solar Program Multi-Year Technical Plan is to reduce the cost solar modules to a level more competitive with traditional fossil fuel based electricity generation. Unfortunately, the crystalline silicon (c-Si) wafers that are the foundation of today's PV industry are likely to have a fundamental lower limit on their cost per unit area. Thus, while silicon appears to be the near-ideal PV material – it is abundant, non-toxic, and benefits from an enormous knowledge base and industrial infrastructure – silicon wafers will eventually prove too expensive. This limitation has stimulated research into growing c-Si films for solar cells but, thus far, no routes to c-Si films have demonstrated the capability to achieve the necessary high conversion efficiencies. The limitations of these other approaches has motivated us to propose a new route to thin film c-Si that will result in films with electronic properties capable of high efficiency PV.

2. Technical Approach

We have developed a new approach to c-Si on glass based on an initial deposition of a foreign template layer to control both the in-plane and out-of-plane orientation of the thin crystal silicon films. The resulting low-angle grain boundaries in the silicon films should be less deleterious to film properties and should permit improved photovoltaic efficiencies. This new template approach relies on the initial deposition of a biaxially textured film and the subsequent templated or heteroepitaxial growth of a c-Si seed layer. Further thickening of the Si seed layer by homoepitaxy or by Si SPE will be simplified by the uniform out-of-plane grain orientation. In this paper, we outline the template approach to biaxially textured c-Si films on glass, describe relevant experimental results and discuss the research challenges that will need to be overcome to

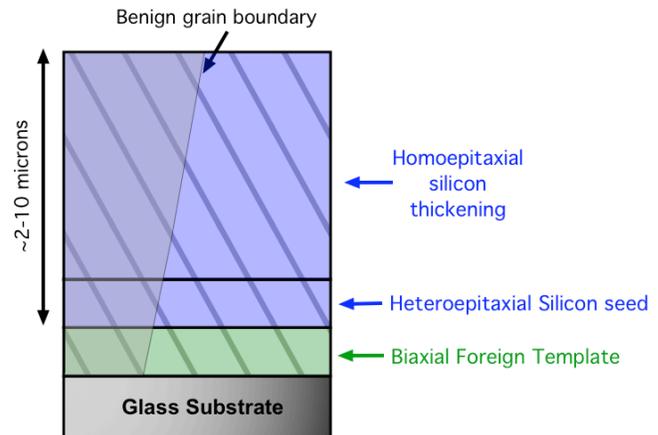


Fig. 1. Proposed structure to grow biaxially textured c-Si films on glass using a biaxially textured foreign template layer.

fabricate films good enough to incorporate in high efficiency devices.

3. Results and Accomplishments

Our approach to c-Si on glass is motivated by the impressive recent results in the superconductor community where they have used "template layers" to transition from a disordered substrate to well-ordered crystalline superconductor films.¹ As shown in Figure 1, we propose to take a similar approach to grow c-Si on glass. We will use ion-beam assisted deposition (IBAD) or inclined substrate deposition (ISD) to grow a biaxially textured template layer on glass and subsequently grow a silicon layer on this template. We anticipate that biaxially textured thin silicon will be much easier to achieve on crystalline template layer than on the initial amorphous substrate. Subsequent thickening of the silicon layer will also be easier, as the silicon seed layer will be uniformly oriented and it will not be necessary to achieve epitaxial silicon growth on different crystalline orientations simultaneously. Recently, Findikoglu et al² showed that c-Si with a total mosaic spread of 2-3° can be grown on template-coated polycrystalline Hastelloy with a maximum processing temperature of 780°C. These c-Si films have Hall mobilities that increase exponentially as the grain-angle disorder is decreased and approach that of single-crystal Si. The challenge will be to achieve similar results on glass at a lower temperature.

3.1 Foreign Template Layer Growth

The most promising approaches to growing a biaxially textured template on glass are to use IBAD or ISD. In the IBAD process, the in-plane deposition symmetry is broken by a collimated beam of ions that is directed at the growing film surface at a selected angle, different from the surface normal. Under the right conditions, the interaction of the ion beam and the growing film results in biaxial texture. With ISD, the depositing atoms themselves are incident at non-normal incidence to the substrate. A useful template material will be readily deposited with biaxial texture on glass and will be compatible with subsequent silicon epitaxy. Ideally, the template would also be conductive, so as to provide a back contact for the solar cell. A large knowledge base already exists for growing biaxially textured thin films of oxides such as Y-stabilized ZrO₂, CeO₂, and MgO³ on amorphous or polycrystalline substrates and any of these cubic materials could be used as template layers for c-Si growth. Of these oxides, CeO₂ has the advantage of being nearly perfectly lattice-matched to silicon ($a_{\text{ceria}}=5.41 \text{ \AA}$ compared to $a_{\text{c-Si}}=5.43 \text{ \AA}$). One challenge in growing the template layer will be obtaining a sufficiently well ordered film rapidly enough to keep manufacturing costs low. MgO is exciting because it develops biaxial texture within about 10 nm of IBAD growth.⁴ We are also looking at other lattice-matched materials such as CoSi₂ by IBAD because the chemical compatibility of the Si/CoSi₂ interface has already been established and because Co is a relatively benign impurity in c-Si.

3.2 Growth of c-Si seed on foreign templates

Epitaxial thin-film growth of silicon has been achieved at glass-compatible temperatures on single crystal wafer substrates by many techniques. However, less research has been done on the epitaxial growth of Si films on foreign crystalline substrates. The greatest challenge is likely to be the high interfacial reactivity of the Si. The best results of silicon epitaxy on foreign substrates have been accomplished under ultra-high vacuum or at temperatures too high to be compatible with glass.^{3,5} A crucial challenge will be growth of epitaxial silicon seed layers at temperatures low enough to be compatible with inexpensive glasses (below 600°C) and at reasonable pressures ($\sim 10^{-7}$ Torr).

Temperature and pressure restrictions are less problematic for solid-phase epitaxy (SPE), where silicon is initially deposited as an amorphous film and then crystallized during a subsequent annealing. A key advantage of solid-phase epitaxy is that it is a simple batch process. We are unaware of any research on Si SPE on foreign materials.

3.4 Initial Experiments at NREL

To-date, work in our laboratory has focused on growth of biaxially-textured CeO₂ films on glass using ion beam assisted deposition and inclined substrate deposition by magnetron sputtering and growing heteroepitaxial silicon films by SPE on single crystal CeO₂ layers.

The CeO₂ films grown on glass using IBAD or directional sputtering have shown biaxial (100) texturing mixed with a small amount of uniaxial (111) texturing. It is likely that the films begin growth with a mixture of textures but that in plane aligned (100) grains increase in size as the film is thickened.

Amorphous silicon films have been deposited onto single crystal CeO₂ using hot-wire CVD. The films were then crystallized by annealing in a furnace for 8 h at 580°C. The TEM measurements also show that an amorphous SiO_x forms about 3 nm thick at the CeO₂/Si interface. We believe that this oxide forms by a rapid reaction of the Si and CeO₂, at the interface. Thus, the crystalline order of the CeO₂ template is disrupted and this prevents the desired heteroepitaxial nucleation of well-oriented silicon grains.

4. Conclusions

We have proposed a new approach to growing c-Si films on glass with electronic properties capable of achieving high PV efficiencies. The key to our approach is the development of in and out-of-plane aligned c-Si grains, achieved through the initial deposition of a biaxially textured template layer.

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